Aerosol modeling with WRF/Chem

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WRF/Chem Tutorial, 31 July 2014
(Valid for WRF/Chem 3.5)
Part I - Introduction

- **Overview of ...**
  - Aerosol
  - Aerosol processes and life cycle
  - Model treatment of aerosol
  - WRF/Chem aerosol schemes

Part II – The details

- **Representing the aerosol size distribution**
- **Walk through the WRF/Chem aerosol schemes**
  - How they work and what they do
  - Coupling to other processes
    - Gas phase chemistry
    - Aqueous chemistry
    - ...
- **Hint on how to tell WRF/Chem what to do**
- **Resources**
Part I – Introduction
Aerosol
Aerosol life cycle and processes

Particle diameter

- ~ 0.3 nm
- ~ 1 nm
- ~ 3 nm
- ~ 3-50 nm
- >50 nm

Processes:

- Nucleation
- Condensation, coagulation
- Activation, aqueous chemistry, wet scavenging
- Loss onto aerosol particles from surface emissions, dry deposition
- Surface emissions

Reactions:

- UV radiation
- OH
- OH + SO₂
- H₂O
- H₂SO₄
- Organic molecules

Chemical reactions:

- OH + SO₂ → H₂SO₄
- Nucleation
- Condensation, coagulation
- Activation, aqueous chemistry, wet scavenging

Surface emissions include:

- H₂O
- H₂SO₄
- Organic molecules

Loss onto aerosol particles includes:

- Dry deposition

Individual processes or sets of processes are treated by “modules” or “schemes”.

Model treatment of aerosol

- Cloud microphysics
- Radiative transfer
- Gas phase chemistry
- Aerosol chemistry
- Aerosol nucleation
- Emissions
- Dry deposition
WRF/Chem aerosol schemes

- **An efficient aerosol scheme from the GOCART model**
  - No size information for sulfate, BC, OC
  - Size information for dust and sea salt
  - No secondary organic aerosol (SOA)

- **Modal Aerosol Dynamics Model for Europe – MADE**
  - 3 log-normal modes
  - Inorganic, organic aerosol, SOA

- **Model for Simulating Aerosol Interactions and Chemistry (MOSAIC)**
  - Sectional model, 4 or 8 bins
  - Inorganic, organic aerosol, SOA

- **MAM – Modal Aerosol Model (new in WRF/Chem 3.5) from CAM5**
  - 3 or 7 log-normal modes
  - Inorganic, organic aerosol, SOA, sea salt, BC, mineral dust

- **Simple sectional (bin) scheme for volcanic ash aerosol**
Part II – The details
• Only total mass of aerosol compounds is known

• No information on
  ▪ Particle number
  ▪ Aerosol size distribution

Aerosol size distribution needs to be assumed for:
  ▪ radiative transfer
  ▪ response of cloud properties to aerosol number

• Numerically efficient
• Useful when focus is on complex gas phase chemistry

→ GOCART (+ size resolved dust and sea salt)
Modal aerosol schemes
Modal aerosol schemes

Twin Otter data (black)

\[ \frac{dN}{dD} = \frac{N}{\sqrt{2\pi \ln(\sigma) D}} e^{-\frac{1}{2} \left( \frac{\ln(D/\mu)}{\ln(\sigma)} \right)^2} \]

\[ \frac{dN}{dD} \rightarrow N = 8195 \text{ cm}^{-3} \]
\[ \mu = 18.22 \text{ nm} \]
\[ \sigma = 1.42 \]

\[ \frac{dN}{dD} \rightarrow N = 12732 \text{ cm}^{-3} \]
\[ \mu = 68.44 \text{ nm} \]
\[ \sigma = 1.57 \]

\[ \frac{dN}{dD} \rightarrow N = 3140 \text{ cm}^{-3} \]
\[ \mu = 164.41 \text{ nm} \]
\[ \sigma = 1.28 \]
Modal aerosol schemes

\[ \frac{dN}{dD} = \frac{dN}{dD} + \frac{dN}{dD} + \frac{dN}{dD} \]

Twin Otter data (black)
Modal aerosol schemes

→ MADE and MAM
Sectional aerosol schemes

→ MOSAIC, volcanic ash, (GOCART)
GOCART aerosol module

- Georgia Tech/Goddard Global Ozone Chemistry Aerosol Radiation and Transport model (Chin et al., JGR, 2000)
  - **Bulk aerosol:**
    - Hydrophobic black carbon (fresh soot)
    - Hydrophilic black carbon (aged/coated soot)
    - Hydrophobic organic carbon (fresh burnt biomass)
    - Hydrophilic organic carbon (aged/coated burnt biomass)
      - Fresh $\rightarrow$ aged conversion time 2.5 days
    - Other GOCART primary PM2.5
    - Other GOCART primary PM10
    - Sulfate (only secondary aerosol species)
  - **Sectional scheme for dust and sea salt:**
    - Dust: 0.5, 1.4, 2.4, 4.5, 8.0 $\mu$m effective radius
    - Sea salt: 0.3, 1.0, 3.2, 7.5 $\mu$m effective radius
GOCART comes with sulfur gas phase chemistry:

- $\text{DMS} + \text{OH} \rightarrow \text{SO}_2 + ...$
- $\text{DMS} + \text{OH} \rightarrow \text{MSA} + ...$
- $\text{DMS} + \text{NO}_3 \rightarrow \text{SO}_2 + ...$
- $\text{SO}_2 + \text{OH} \rightarrow \text{SO}_4^2- + ...$

Extended gas phase chemistry can be used:

- MOZART (with KPP)
- RACM (with KPP)
- RADM (with and without KPP)
• **Interaction with radiation:**
  - Direct effect for some model setups
  - Effect on photochemistry

• **Interaction with clouds:**
  - Aqueous chemistry
    - $\text{SO}_2 + \text{H}_2\text{O}_2 \rightarrow \text{SO}_4^-$
    - $\text{SO}_2 + \text{O}_3 \rightarrow \text{SO}_4^-$
  - No indirect effect
  - No wet scavenging/deposition

• **No secondary organic aerosol (SOA)**
MADE aerosol module

Modal Aerosol Dynamics Model for Europe
(Ackermann et al., Atm. Env., 1998)

- 3 log-normal aerosol modes: Aitken, accumulation, coarse
- Mode width $\sigma$ is fixed
- Aerosol number and mass variable
- (Currently no nucleation mode)

Interaction with radiation:
- Direct aerosol effect
- Effect on photolysis

Interaction with clouds:
- Aerosol number determines cloud drop number and size
- Radiative response $\rightarrow$ 1st indirect aerosol effect
  - only for resolved clouds (Sc)
- Aqueous chemistry
- Wet removal (scavenging)
Aitken and accumulation modes:

- $\text{SO}_4^-$, $\text{NH}_4^+$, $\text{NO}_3^-$, $\text{H}_2\text{O}$
- NaCl (sea salt)
- Anthropogenic SOA from oxidation of...
  - Alkanes
  - Alkenes
  - Aromatics
- Biogenic SOA from oxidation of...
  - Alpha-pinene
  - Limonene
  - Isoprene
- Anthropogenic POA
- Elemental carbon (soot)
- Primary PM2.5
MADE aerosol module

Coarse mode:

- Anthropogenic primary aerosol – e.g. from
  - Coal combustion
  - Cement manufacturing
  - Metallurgy
  - Waste incineration
- Sea salt
- Soil derived particles (mineral dust)
MADE aerosol coupling with chemistry

- **Gas phase chemistry:**
  - RADM2 *(Regional Acid Deposition Model version 2)*
  - RACM *(Regional Atmospheric Chemistry Mechanism)*
  - RACM NOAA/ESRL version
  - CBMZ *(Carbon-Bond Mechanism version Z)*

- **Gas phase/particle partitioning (aerosol chemistry):**
  - MARS *(Model for an Aerosol Reacting System)*
  - SORGAM *(Secondary Organic Aerosol Model)*
  - VBS *(Volatility Basis Set)*

- **Aqueous chemistry:**
  - CMU aqueous chemistry
  - CMAQ *(EPA) aqueous chemistry*
  - Only for Aitken and accumulation mode
  - Only for selected gas phase chemistry options
MADE and MARS: Inorganic aerosol chemistry

\[
\begin{align*}
\text{H}_2\text{O} & \\
\text{H}_2\text{SO}_4 & \\
\text{NH}_3 & \\
\text{HNO}_3 & \\
\text{NH}_4\text{HSO}_4 & \\
\text{SO}_3 = & \\
\text{H}_3\text{O}^+ & \\
\text{H}_2\text{O} & \\
\text{SO}_4 & \\
\text{NaCl} & \\
\text{NO}_3^- & \\
\text{SOA} & \\
\text{NH}_4^+ & \\
\text{NH}_3 & \\
\end{align*}
\]

MARS (Model for an Aerosol Reacting System), Saxena et al., Atm. Env., 1986
MADE/SORGAM

Gas phase scheme (RADM2, RACM)

<table>
<thead>
<tr>
<th>Alkanes</th>
<th>Alkenes</th>
</tr>
</thead>
</table>
| Toluene          | Xylene, cresole, ...
|                  |                  |

- Alkanes
- Alkenes
- Toluene
- Xylene, cresole, ...

Isoprene

Sesquiterpene

Alpha-pinene, limonene

**Semi-volatile organics**

\[ X_1, X_2, X_3, X_4, X_5, \ldots, X_n \]

**SOA**

\[ \text{H}_3\text{O}^+, \text{HSO}_4^- \]

\[ \text{NH}_4\text{HSO}_4 \]

\[ \text{H}_2\text{O} \]

\[ \text{SO}_4^{2-} = (\text{NH}_4)_2\text{SO}_4 \]

\[ \text{NO}_3^- \]

\[ \text{SO}_3^- \]

\[ \text{NH}_4^+ \]

\[ \text{NaCl} \]

**SORGAM** (Secondary Organic Aerosol Model), Schell et al., JGR, 2001
MADE/VBS (Volatility Basis Set)

Gas phase scheme (RACM)

- Alkanes
- Alkenes
- Toluene
- Xylene, cresole, ...
- Isoprene
- Sesquiterpene
- Alpha-pinene, limonene

Products

- Volatile
- Semi-volatile

Volatility

$\text{OH, O}_3, \text{NO}_3$

Ahmadov et al., JGR 2012
MADE/VBS (Volutatility Basis Set)

Organic aerosol mass in the surface layer
(August - September 2006)

Ahmadov et al., JGR 2012
MADE and aqueous chemistry

- **CMU aqueous chemistry** (Fahey & Pandis, Atm. Env., 2001)
  - Slow
  - Only for resolved clouds (Sc)
  - Does not really conserve mass

- **CMAQ aqueous chemistry** (Walcek & Taylor, JAS, 1986)
  - Relatively fast
  - In both resolved (Sc) and parameterized (Cu) clouds
  - Coupled to wet deposition of $\text{SO}_4^{2-}$ and $\text{NO}_3^-$

MADE + CMAQ aqueous chemistry + wet deposition of $\text{SO}_4^{2-}$ and $\text{NO}_3^-$:

- `chem_opt = 41` : RADM2 gas phase chemistry

Planned for WRF/Chem 3.5.1:

- `chem_opt = 42` : RACM gas phase chemistry (KPP)
- `chem_opt = 43` : RACM ESRL gas phase chemistry (KPP)
MADE and CMAQ aqueous chemistry

Details of aqueous chemistry depend on cloud type

Stratocumulus

Cumulus

Cumulonimbus

~10km

~100m

~1km
MADE and wet deposition

Precipitation

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<tbody>
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SO$_4^-$ wet dep.

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<th>r</th>
<th>model/obs.</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.86</td>
<td>0.53</td>
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</table>

May-September 2006
(National Atmospheric Deposition Program)
MOSAIC aerosol module

Model for Simulating Aerosol Interactions and Chemistry (Zaveri et al., JGR, 2008)

- Modern aerosol scheme in WRF/Chem
- 4 or 8 aerosol size sections (bins) 39 nm – 10 μm
- (Lower bin boundary of 39 nm too large for nucleation)
- Interaction with radiation:
  - Direct aerosol effect
  - Effect on photolysis
- Interaction with clouds:
  - Aerosol number determines cloud drop number and size
  - Radiative response → 1st indirect aerosol effect
  - Aqueous chemistry
  - Wet removal (scavenging)
  - only for resolved clouds (Sc)
MOSAIC aerosol module

Aerosol composition

- $\text{SO}_4^{2-}$, $\text{NH}_4^+$, $\text{NO}_3^-$, $\text{H}_2\text{O}$
- $\text{NaCl}$ (sea salt)
- $\text{CH}_3\text{SO}_3$ (methanesulfonate)
- carbonate ($\text{CO}_3^-$)
- calcium (Ca)
- black carbon (BC)
- primary organic mass (OC)
- other inorganic mass (minerals, trace metals)
MOSAIC aerosol coupling with chemistry

- **Gas phase chemistry:**
  - CBMZ (Carbon-Bond Mechanism version Z)
    - “Standard” gas phase chemical scheme for MOSAIC
  - SAPRC99 (extensive VOC chemistry)
  - MOZART (Model for Ozone and Related chem. Tracers)
  - Works with the VBS SOA scheme

- **Gas phase/particle partitioning (aerosol chemistry):**
  - MTEM (Multicomponent Taylor Expansion Method)
  - MESA (Multicomponent Equilibrium Solver for Aerosols)
  - VBS (Volatility Basis Set)

- **Aqueous chemistry:**
  - CMU aqueous chemistry, only for resolved clouds (Sc)
  - Not with KPP versions of gas phase chemistry schemes
MOSAIC, MTEM, and MESA

MTEM calculates activity coefficients
MESA solves ion-equilibria in the liquid phase
For SOA: VBS (Volatility Basis Set) scheme

MTEM (Multicomponent Taylor Expansion Method), Zaveri et al., JGR 2005a
MESA (Multicomponent Equilibrium Solver for Aerosols), Zaveri et al., JGR 2005b
Modal Aerosol Model from CAM5

- New in WRF/Chem 3.5
- 3 or 7 log-normal aerosol modes: MAM3 and MAM7
- Mode width $\sigma$ is fixed
- Aerosol number and mass variable
- Liu et al., Geosci. Model Dev., 5, 709-739, 2012
MAM 3

Aitken mode

- Sulfate (SO$_4^{2-}$)
- SOA
- Sea salt

Accumulation mode

Coagulation, condensation

- Sulfate (SO$_4^{2-}$)
- SOA
- Primary organic matter
- Sea salt
- Black carbon
- Mineral dust
- Sea salt

Coarse mode

- Sulfate (SO$_4^{2-}$)
- Mineral dust
- Sea salt

15 – 53 nm
58 – 270 nm
0.8 – 3.65 μm

Dry particle diameter
**MAM 7**

**Aitken mode**
- Sulfate ($SO_4^{=}$)
- SOA
- Sea salt

**Accumulation mode**
- Sulfate ($SO_4^{=}$)
- SOA
- Primary organic matter
- Sea salt
- Black carbon

Coagulation, condensation

- Fine sea salt, $SO_4^{=}$
- Coarse sea salt, $SO_4^{=}$
- Fine dust, $SO_4^{=}$
- Coarse dust, $SO_4^{=}$
MAM aerosol module

- Currently only one gas phase chemistry scheme
  - CBMZ (Carbon-Bond Mechanism version Z)

- Interaction with radiation:
  - Coupled to RRTMG radiation $\rightarrow$ Direct aerosol effect

As in CAM5:

- Gas phase/particle partitioning (aerosol chemistry):
  - Condensation of water vapor and of the 4 inorganic trace gas species: $\text{NH}_3$, $\text{H}_2\text{SO}_4$, $\text{HNO}_3$, $\text{HCl}$

- Interaction with clouds only resolved clouds (Sc):
  - Coupled to Morrison & Gettelman cloud microphysics
  - Radiative response $\rightarrow$ 1$^{\text{st}}$ indirect aerosol effect
  - Wet removal (scavenging)
  - Aqueous chemistry

- Dry deposition
Volcanic ash

- 10 bins for volcanic ash aerosol
- Transport, settling, dry deposition
- Currently no other aerosol
- Single active volcano
- Database of 1535 volcanoes (latitude, longitude, height)
How to tell WRF/Chem what to do

..WRFV3/test/em_real/real.exe
| ../WRFV3/test/em_real/namelist.input
..WRFV3/test/em_real/...
..WRFV3/test/em_real/...

... ...
...
&chem
chem_opt = 42
photdt = 0.25
chemdt = 0
...
...
aerchem_onoff = 1
...
...
conv_tr_aqchem = 1

MADE/SORGAM, RACM, CMAQ aqueous chemistry
Switches all aerosol processes on/off
CMAQ aqueous chemistry on in Cu
Resources

- **WRF/Chem User's Guide**
  - Model options (namelist parameters)
  - Combinations of physical/chemical schemes
  - ...
- **Papers referenced in the WRF/Chem User's Guide**
- **WRF/Chem source code**

- **WRF/Chem Help** (wrfchemhelp.gsd@noaa.gov)
- **Yours truly** (jan.kazil@noaa.gov)